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The Main Characteristics of the Wills-Harrison Effective Pair Potential in Liquid Fe

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Abstract

It is found that the position of the first minimum of the Wills-Harrison effective pair potential in liquid Fe begins to shift significantly to the right-hand side when the *d*-*d*-non-diagonal coupling begins to predominate in the metal under consideration.

Keywords: Transition metal, Wills-Harrison pair potential, *d*-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability p that all 25 *d*-*d* couplings between two different atoms are equiprobable and probability $(1-p)$ that only 5 equiprobable diagonal couplings are possible.

Here, we consider how the magnitude p influences the position, $r_{\min}$, and the magnitude of the first minimum of the WH effective pair potential, $\varphi_{\mathrm{WH}}(r)$, in liquid Fe.

We use the local Bretonnet-Silbert (BS) model pseudopotential [3] for description the *s*-electron contribution to $\varphi_{\mathrm{WH}}(r)$. Input data (WH and BS parameters and the experimental mean atomic volume, Ω) are listed in Table 1.

Figure 2 shows that magnitude of the first minimum quite monotonously increases with increasing p for pair potential under consideration. At the same time, as follows from Figure 1, the first-minimum position begins to increase harshly from $p = 0.6$ approximately. Since the portion of the non-diagonal *d*-*d* couplings in a metal is equal to $0.8p$, it denotes that significant shift of the

$\varphi_{WH}(r)$ first minimum to the right is occurred when the non-diagonal coupling begins to predominate in liquid Fe.

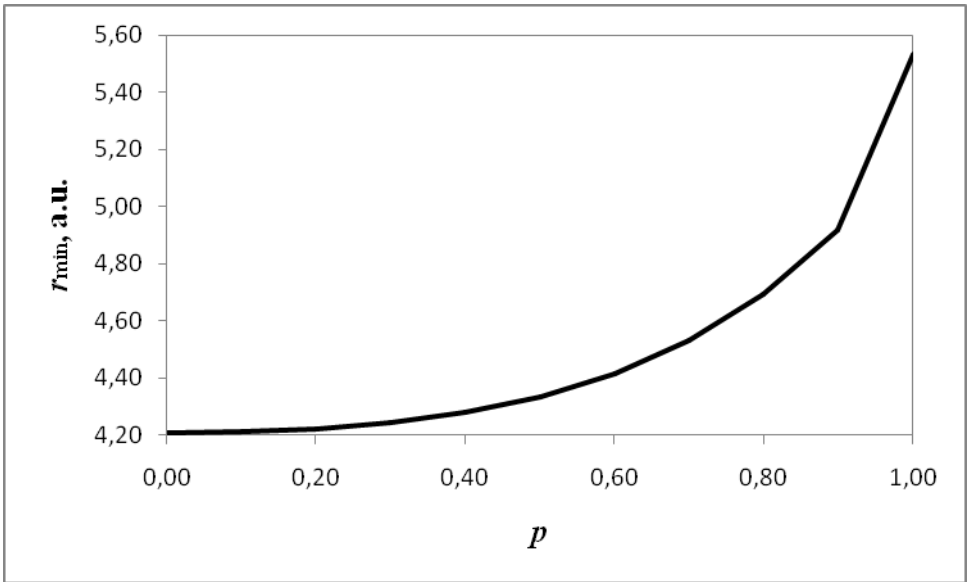

Figure 1. r_{min} of $\varphi_{WH}(r)$ in liquid Fe at different *p* (*T*=1863K).

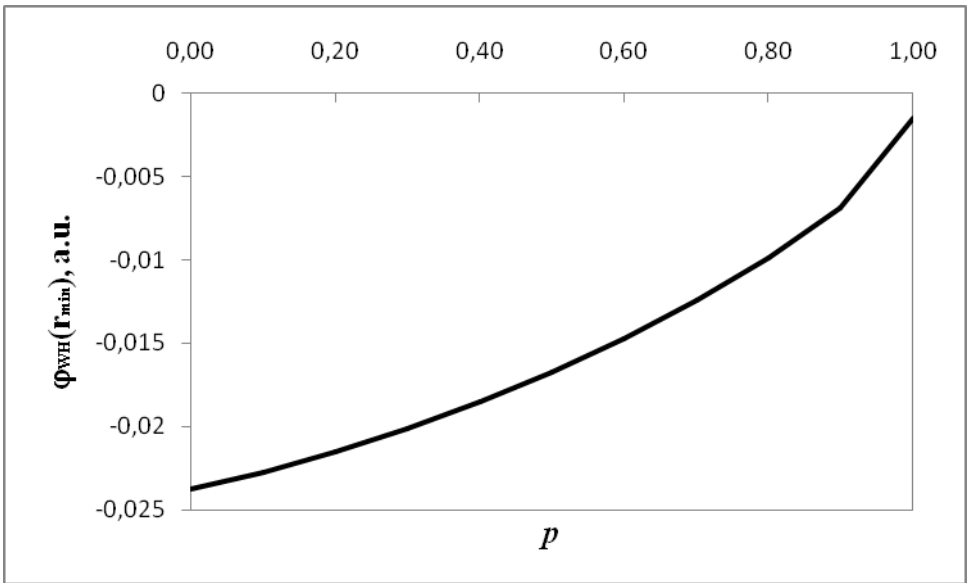

Figure 2. $\varphi_{WH}(r_{min})$ in liquid Fe at different *p* (*T*=1863K).

Table 1. Input data for calculation

r_d (a.u.) [2]	z_s [4]	z_d [4]	R_C (a.u.) [4]	a (a.u.) [4]	Ω (a.u.) [5]
1.512	1.4	6.6	1.54	0.363	89.29

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